Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Highly Soluble Copper(I) Iodide Based Hybrid Luminescent Semiconductors Containing Molecular and One-dimensional Coordinated Anionic Inorganic Motifs

Xiuze Hei,[a] Simon J. Teat,[b] Mingxing Li, [c] Megan Bonite [a] and Jing Li *[a]

[a] *Department of Chemistry and Chemical Biology, Rutgers University, 610 Taylor Road, Piscataway, NJ, 08854, USA*

[b] *Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA*

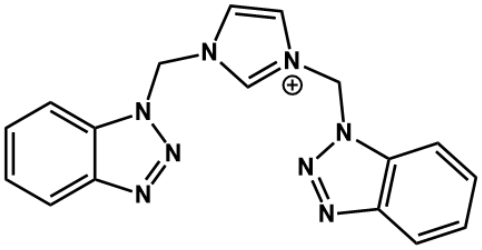
[c] *Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, NY 11973, USA*

TABLE OF CONTENT

S1. Molecular structures and ^{1}H NMR spectra of the ligands.

All the ^{1}H NMR spectra were collected using dimethyl sulfoxide-d6 as solvent. The peaks at 2.50 ppm and ~3.3 ppm are the residue DMSO and water peaks, respectively.

(a)



1,3-bis((1H-benzo[d][1,2,3]triazol-1-yl)methyl)-1H-imidazol-3-ium Iodide
(***L*** $_1$ **I)**

(b)

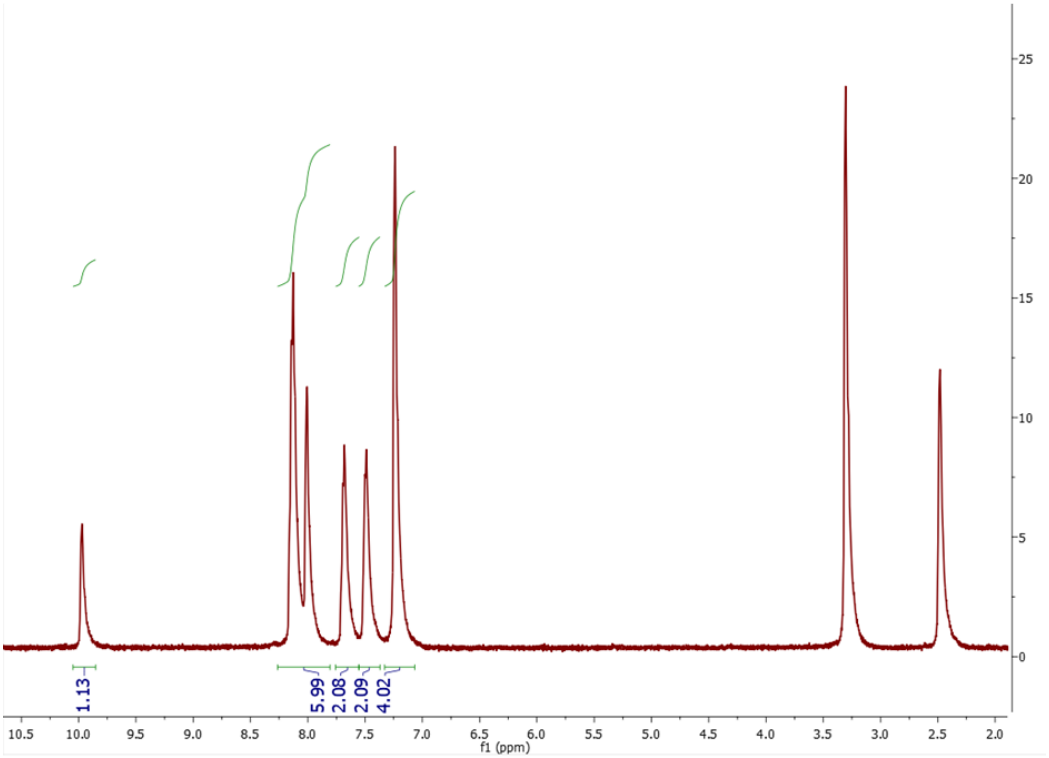
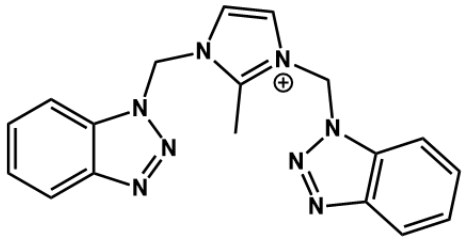


Figure S1. Structural plot and ^{1}H NMR spectrum of L_1 I.

(a)



1,3-bis((1H-benzo[d][1,2,3]triazol-1-yl)methyl)-2-methyl-1H-imidazol-3-ium Iodide

(L_2 I)

(b)

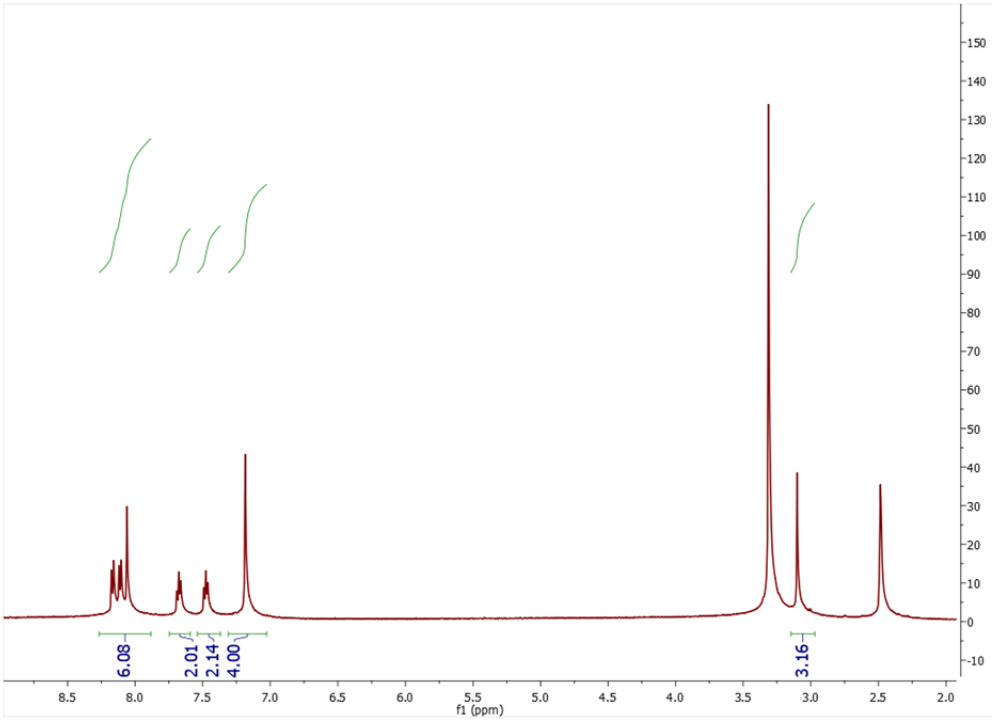
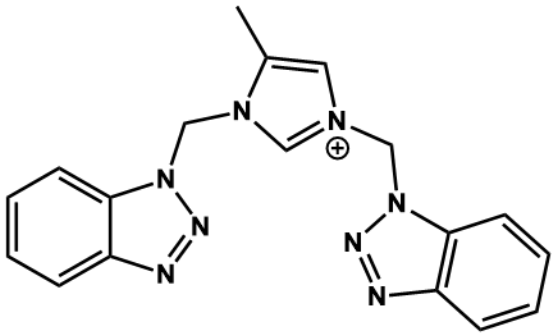


Figure S2. Structural plot and ^{1}H NMR spectrum of L_2 I.

(a)



1,3-bis((1H-benzo[d][1,2,3]triazol-1-yl)methyl)-4ethyl-1H-imidazol-3-ium Iodide

(L_3 I)

(b)

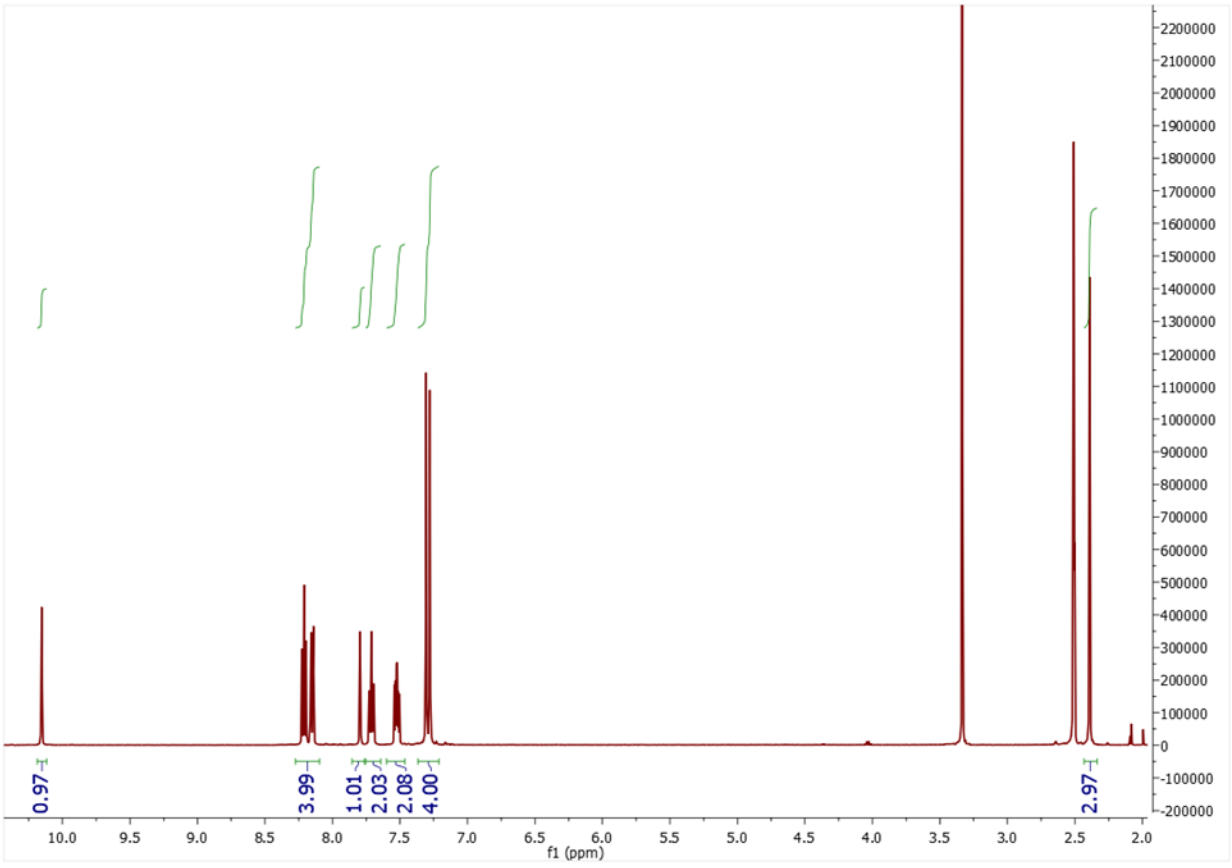
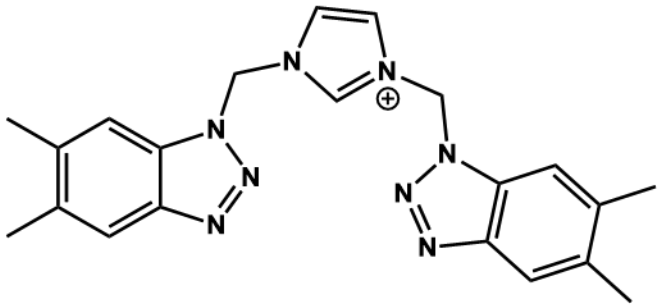


Figure S3. Structural plot and ^{1}H NMR spectrum of L_3 I.

(a)



1,3-bis((5,6-dimethyl-1H-benzo[d][1,2,3]triazol-1-yl)methyl)-1H-imidazol-3-ium Iodide
(*L*$_4$ I)

(b)

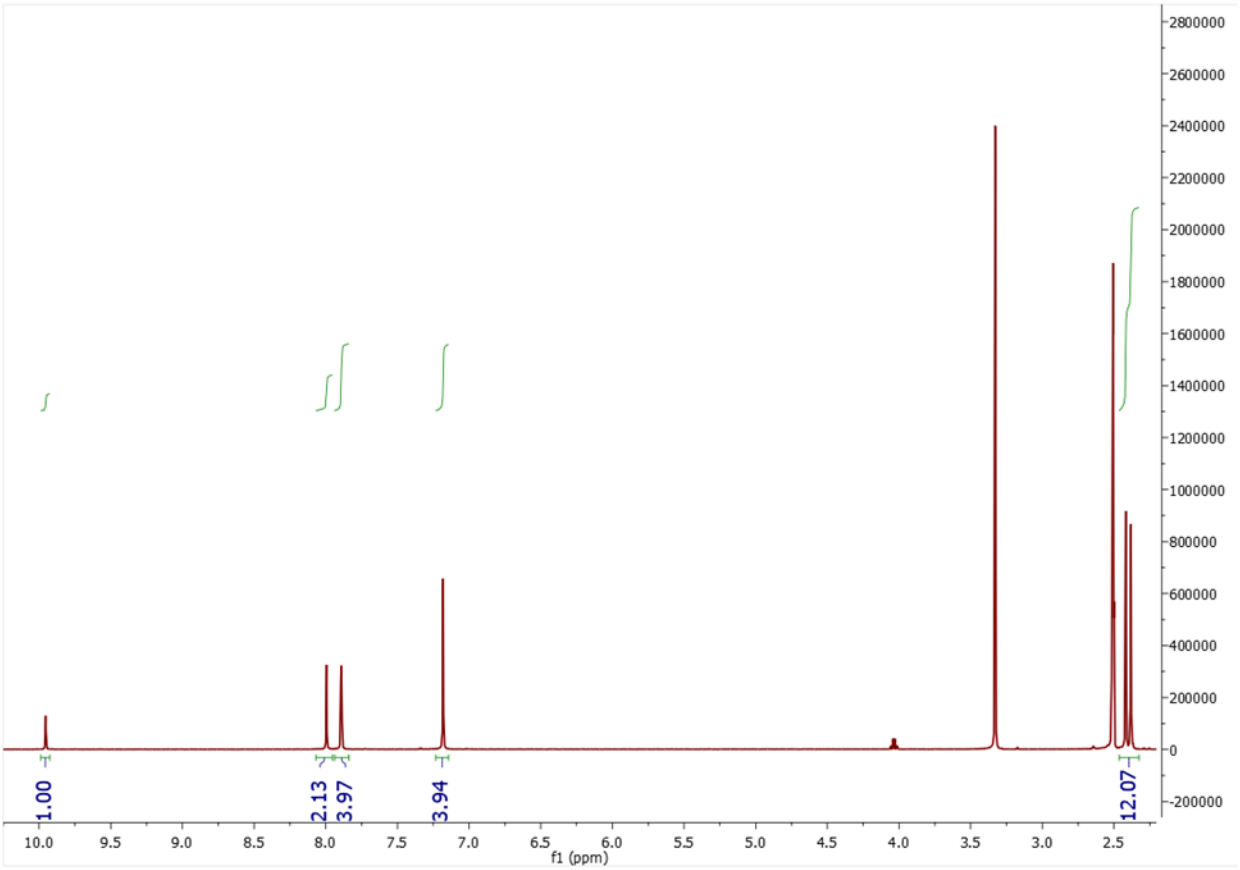


Figure S4. Structural plot and ^{1}H NMR spectrum of *L*$_4$ I.

S2. Structural plots and PXRD patterns of compounds 1-5.

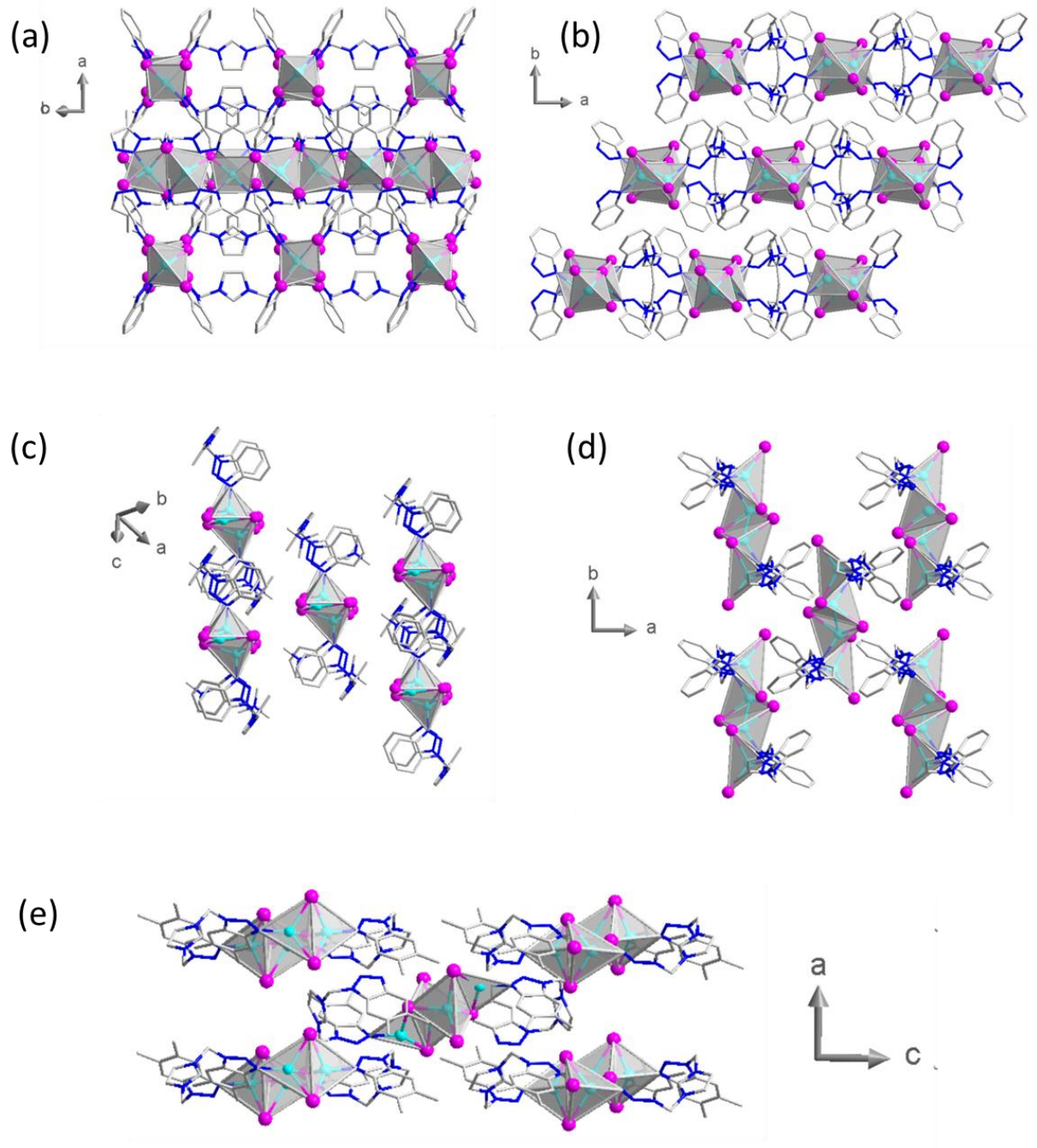


Figure S5. Structure plots of compounds (a) **1**, (b) **2**, (c) **3,** (d) **4** and (e) **5**. All H atoms are omitted for clarity.

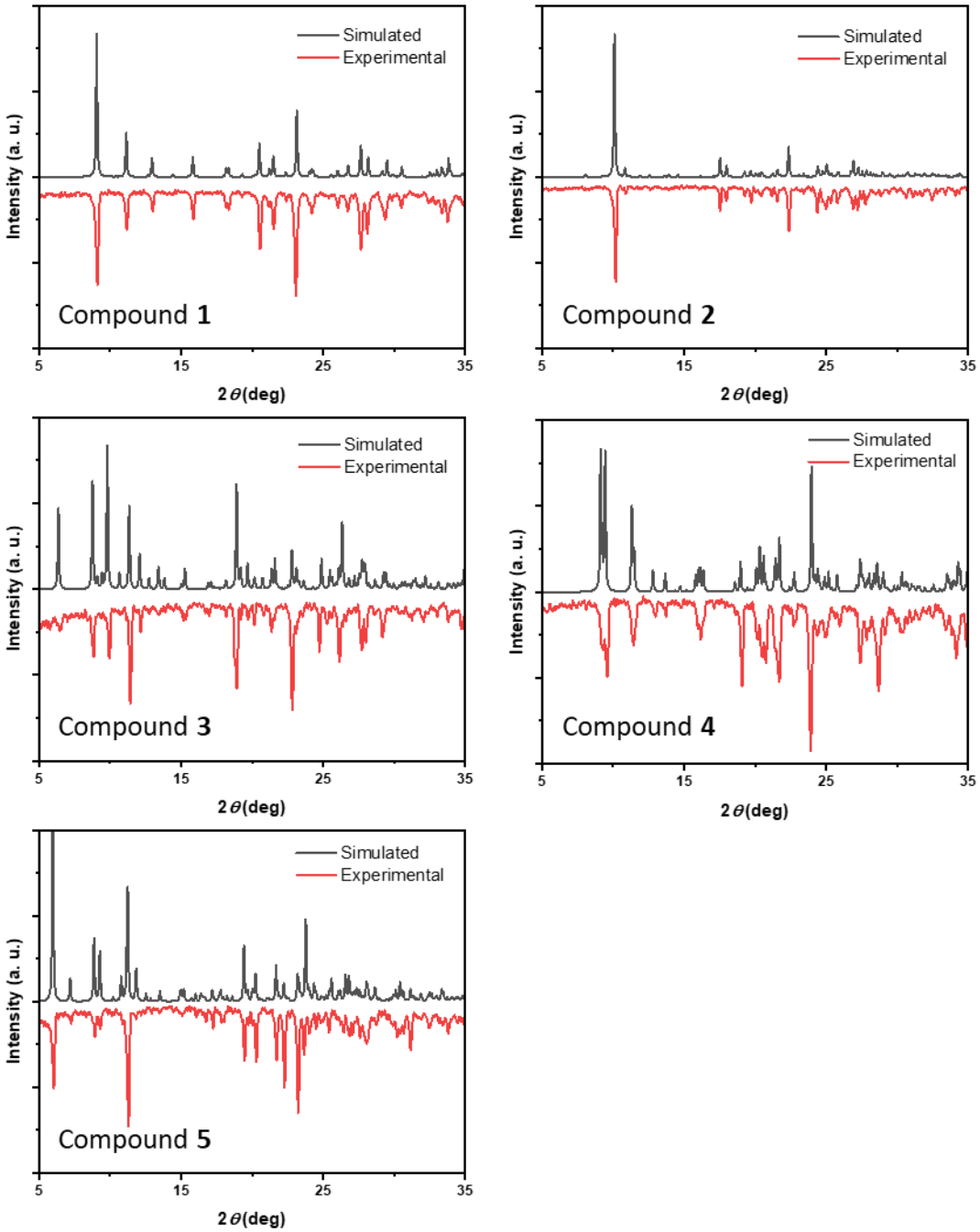


Figure S6. Experimental and simulated PXRD patterns for all five compounds.

S3. Photophysical properties of compounds 1-5.

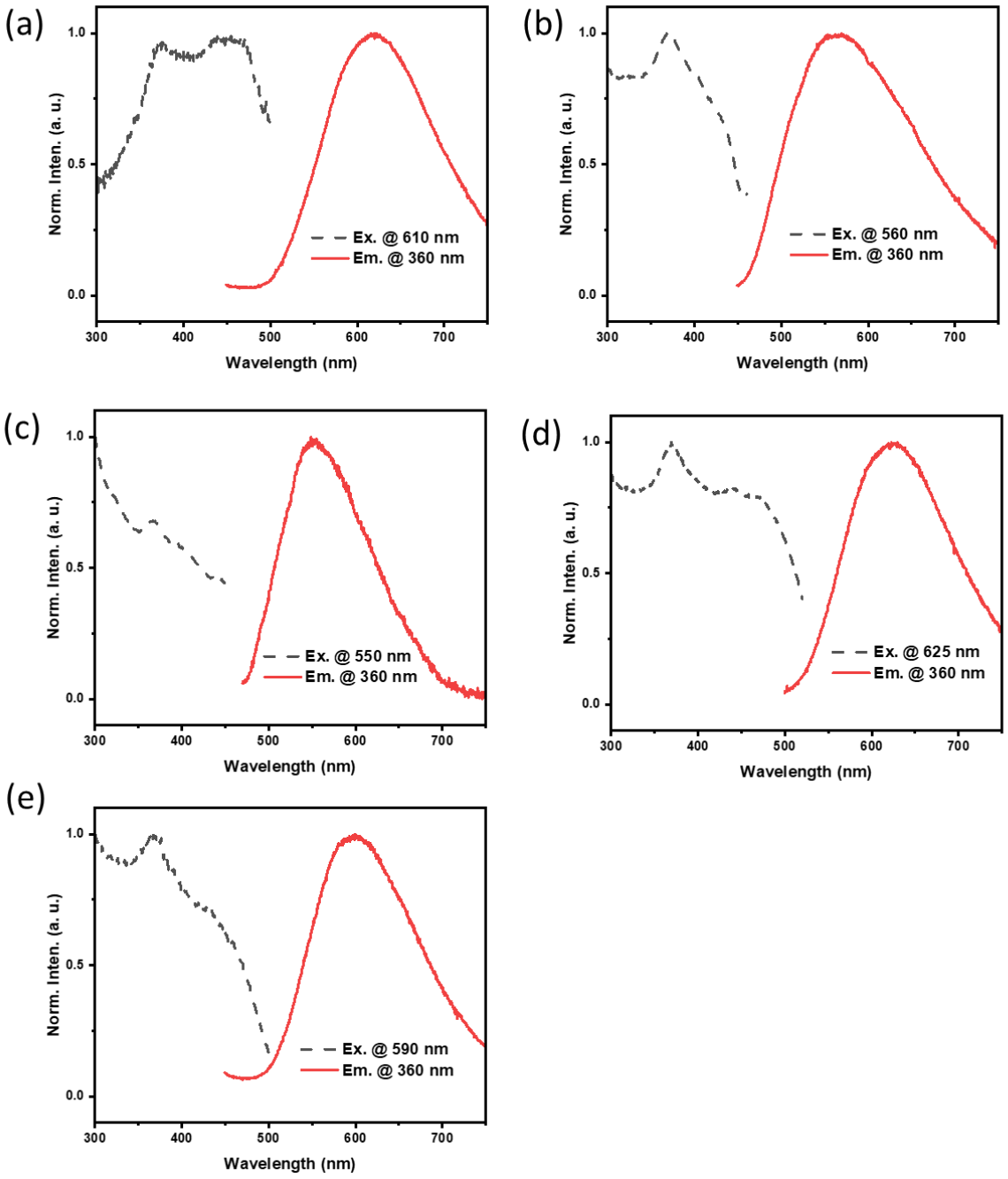


Figure S7. PL and PLE spectra of compounds (a) **1**, (b) **2**, (c) **3,** (d) **4** and (e) **5**.

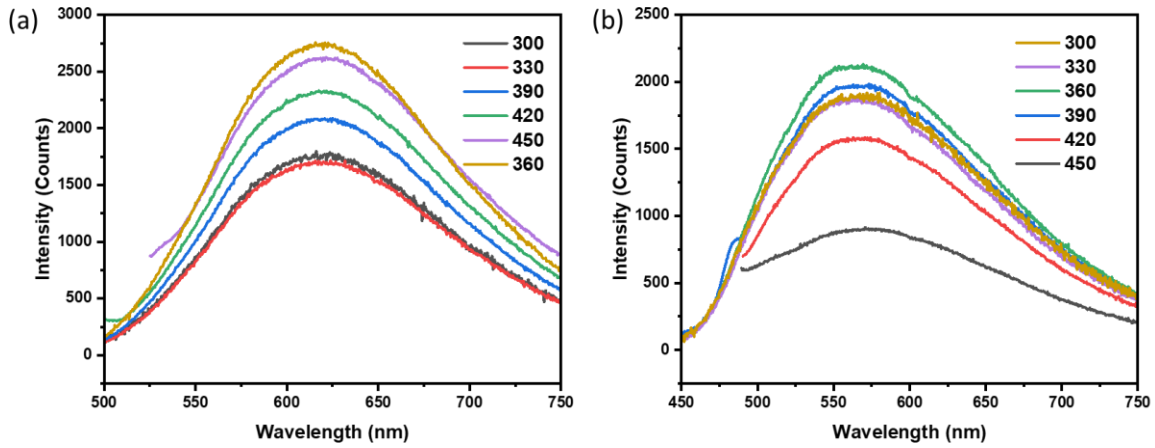
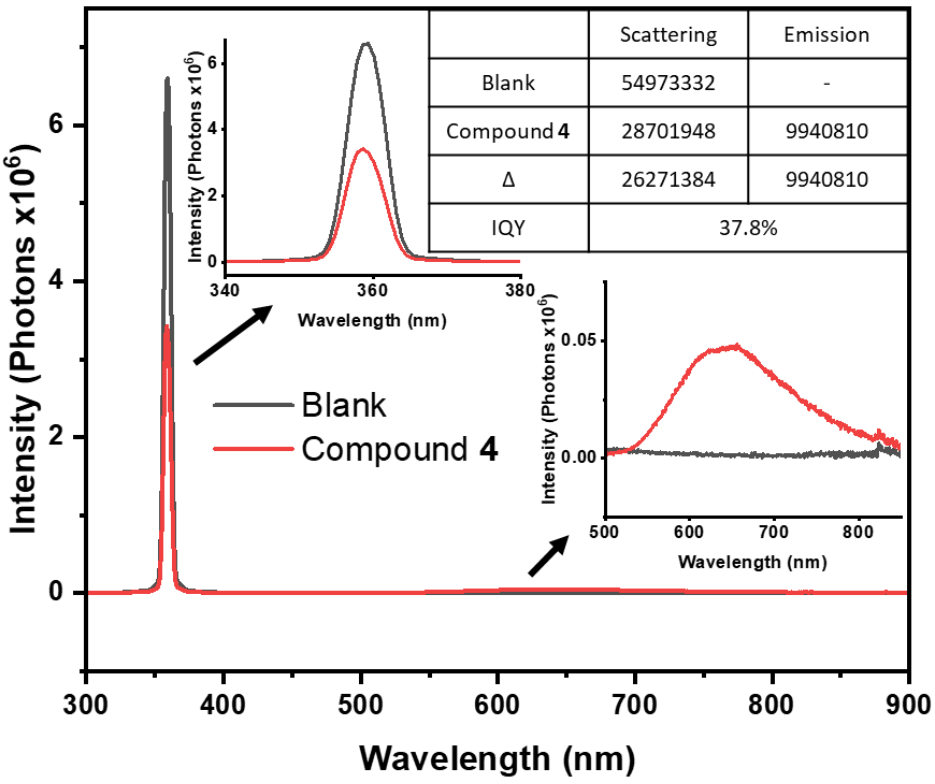
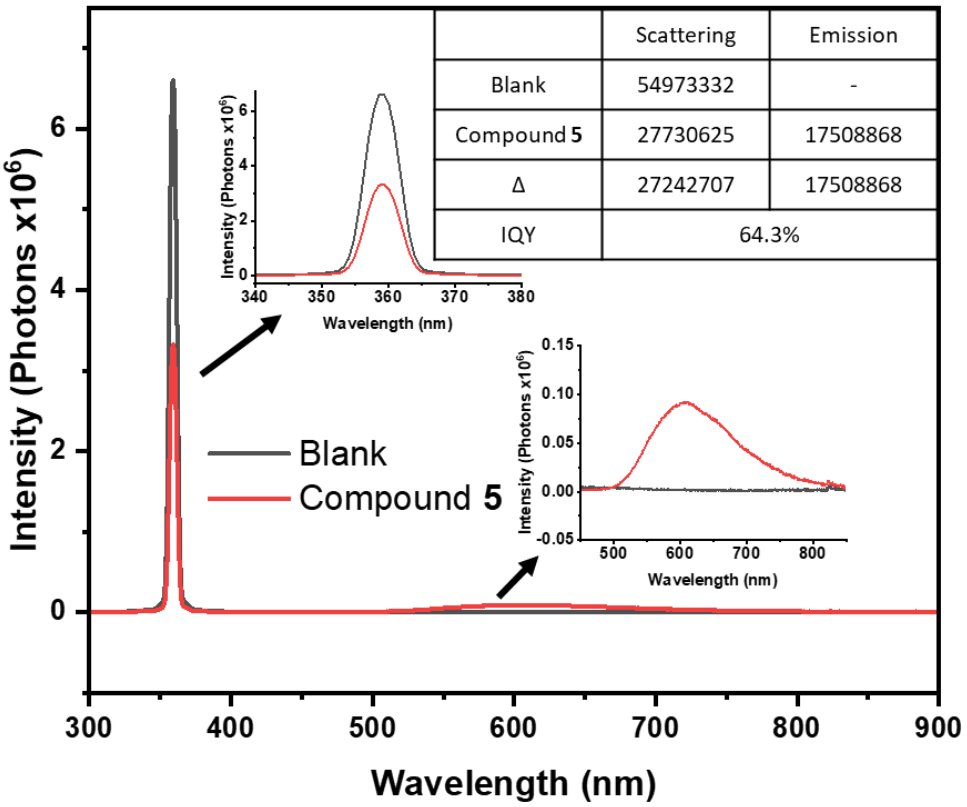


Figure S8. Excitation-dependent PL spectra of (a) compound **1** and (b) compound **2**.



	Scattering	Emission
Blank	54973332	-
Compound **4**	28701948	9940810
Δ	26271384	9940810
IQY	37.8%	

Figure S9. IQY measurement details of compound **4** recorded in the integrating sphere at λ_{ex} = 360 nm.



	Scattering	Emission
Blank	54973332	-
Compound **5**	27730625	17508868
Δ	27242707	17508868
IQY	64.3%	

Figure S10. IQY measurement details of compound **5** recorded in the integrating sphere at λ_{ex} = 360 nm.

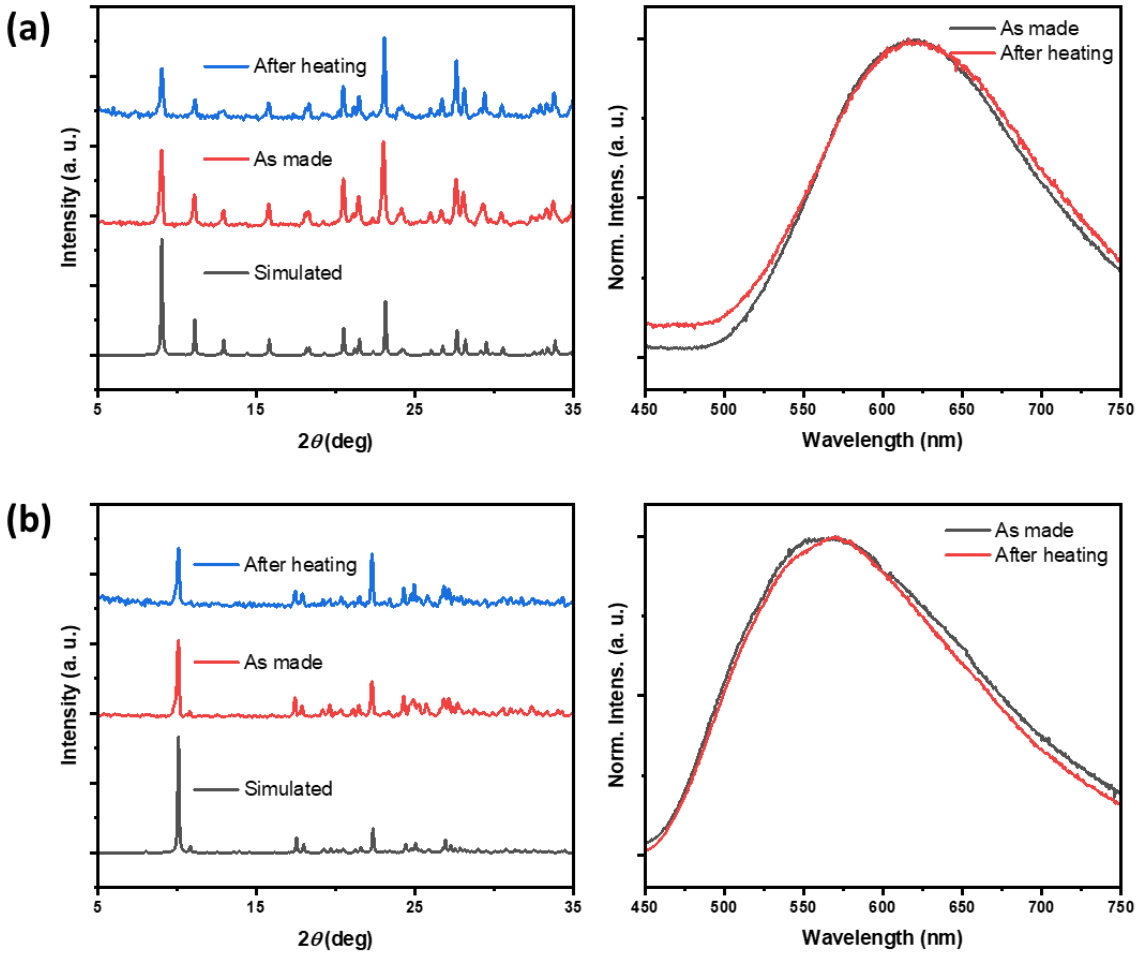


Figure S11. PXRD patterns (left) and PL spectra of (a) compound **1** and (b) compound **2** after heating to 200 °C.

Table S1. Lifetime values of compound **1** at various temperatures.

Temp (K)	A1	τ1 (μs)	A2	τ2 (μs)	τav/int (μs)	τav/amp (μs)
78	235.9 (27.34%)	3.865	626.9 (72.66%)	14.549	13.578	11.628
150	538.1 (49.72%)	3.747	544.1 (50.28%)	11.701	9.788	7.746

200	1220.0 (66.97%)	2.0820	601.6 (33.03%)	7.044	5.1844	3.7207
250	1618.7 (76.83%)	1.0336	488.3 (23.17%)	3.839	2.5157	1.6836
300	2102 (82.66%)	0.4867	440.8 (17.34%)	1.7449	1.0267	0.7048

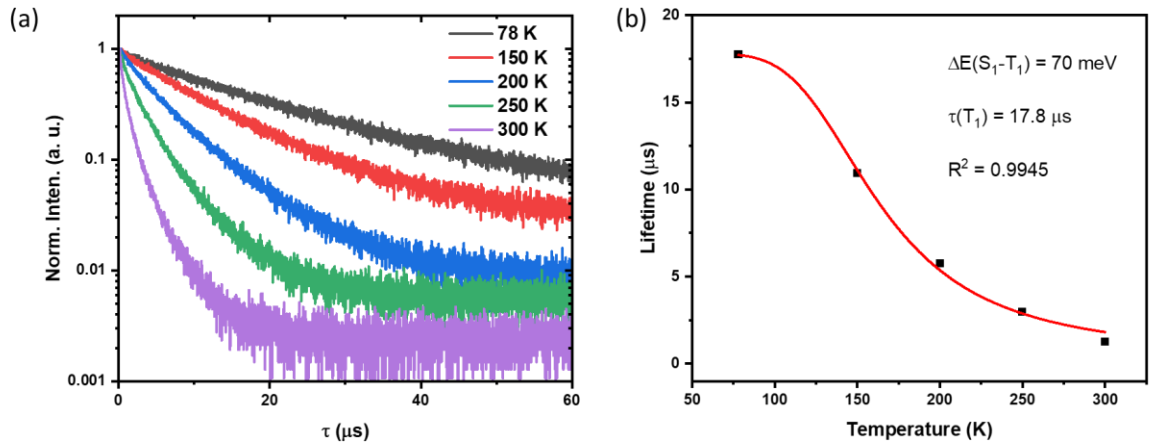


Figure S12. (a) Temperature dependent luminescence decay curves of compound **2**. (b) The observed decay times of compound **2** and the fitting curve according to eq. 1.

Table S2. Lifetime values of compound **2** at various temperatures.

Temp (K)	A1	τ1 (μs)	A2	τ2 (μs)	τav/int (μs)	τav/amp (μs)
78	113.7 (11.46%)	5.16	878.5 (88.54%)	19.392	18.919	17.761
150	795.4 (58.83%)	8.140	556.7 (41.17%)	14.883	11.925	10.916
200	1450.8 (53.29%)	3.442	1271.7 (46.71%)	8.364	6.791	5.741

250	2043.5 (62.74%)	1.7606	1213.8 (37.26%)	5.0373	3.8235	2.9817
300	3036 (75.76%)	0.7389	971.7 (24.24%)	2.8966	1.9396	1.2620

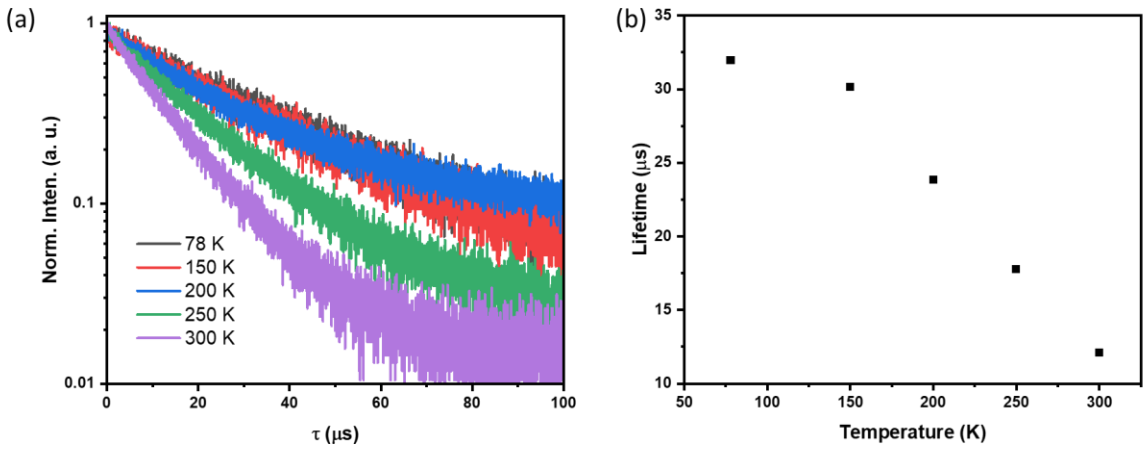


Figure S13. (a) Temperature dependent luminescence decay curves of compound **4**. (b) The observed decay times of compound **4**.

Table S3. Lifetime values of compound **4** at various temperatures.

Temp (K)	**A1**	**τ1 (μs)**	**A2**	**τ2 (μs)**	**τav/int (μs)**	**τav/amp (μs)**
78	26.8 (10.47%)	8.60	229.43 (89.53%)	34.700	33.96	31.97
150	31.8 (13.07%)	8.77	211.83 (86.93%)	33.374	32.44	30.16
200	59.1 (12.47%)	6.94	414.99 (87.53%)	26.238	25.54	23.83
250	54.8 (8.97%)	3.54	556.67 (91.03%)	19.152	18.87	17.75
300	68.2 (9.47%)	3.19	652.4 (90.53%)	13.015	12.77	12.09

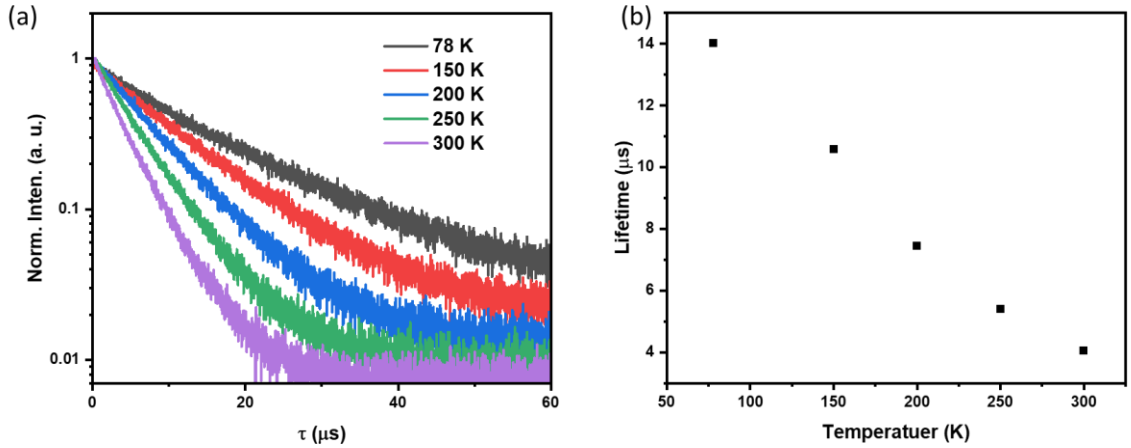


Figure S14. (a) Temperature dependent luminescence decay curves of compound **5**. (b) The observed decay times of compound **5.**

Table S4. Lifetime values of compound **5** at various temperatures.

Temp (K)	A1	τ1 (μs)	τav/int (μs)	τav/amp (μs)
78	865.5	14.029	14.029	14.029
150	880.8	10.575	10.575	10.575
200	1799.5	7.4369	7.4369	7.4369
250	2390.4	5.3924	5.3924	5.3924
300	2837.5	4.0598	4.0598	4.0598

S4. DFT calculations.

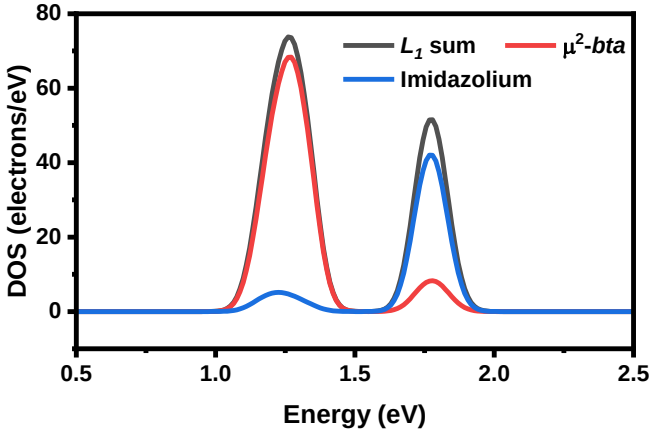


Figure S15. Zoom in of the conduction band region of compound **1**.

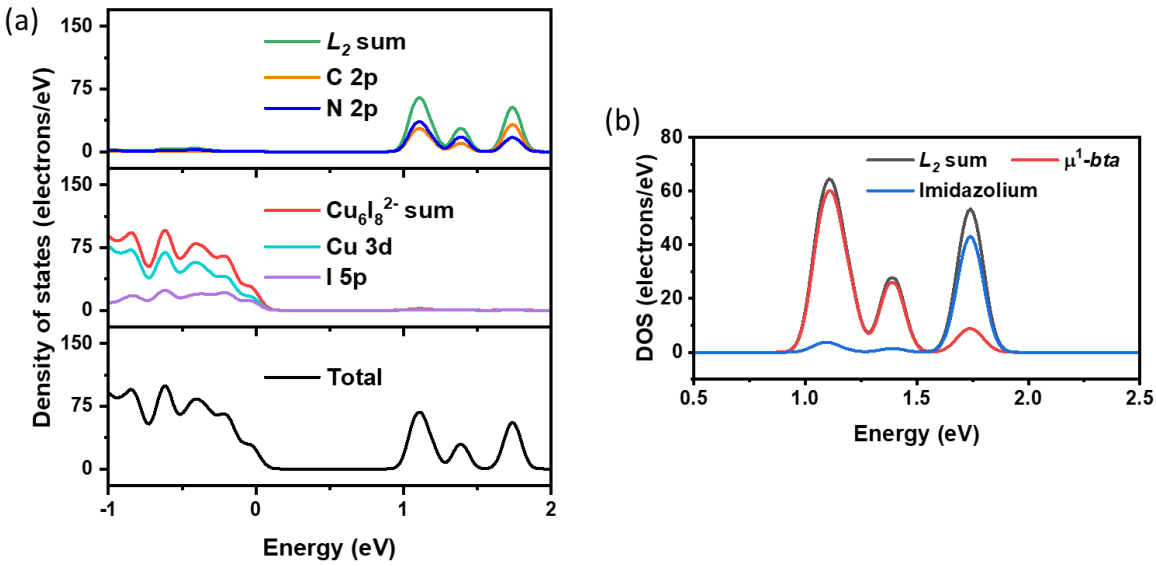


Figure S16. (a) Calculated TDOS and PDOS of compound **2**. (b) Zoom in of the conduction band region of compound **2**.

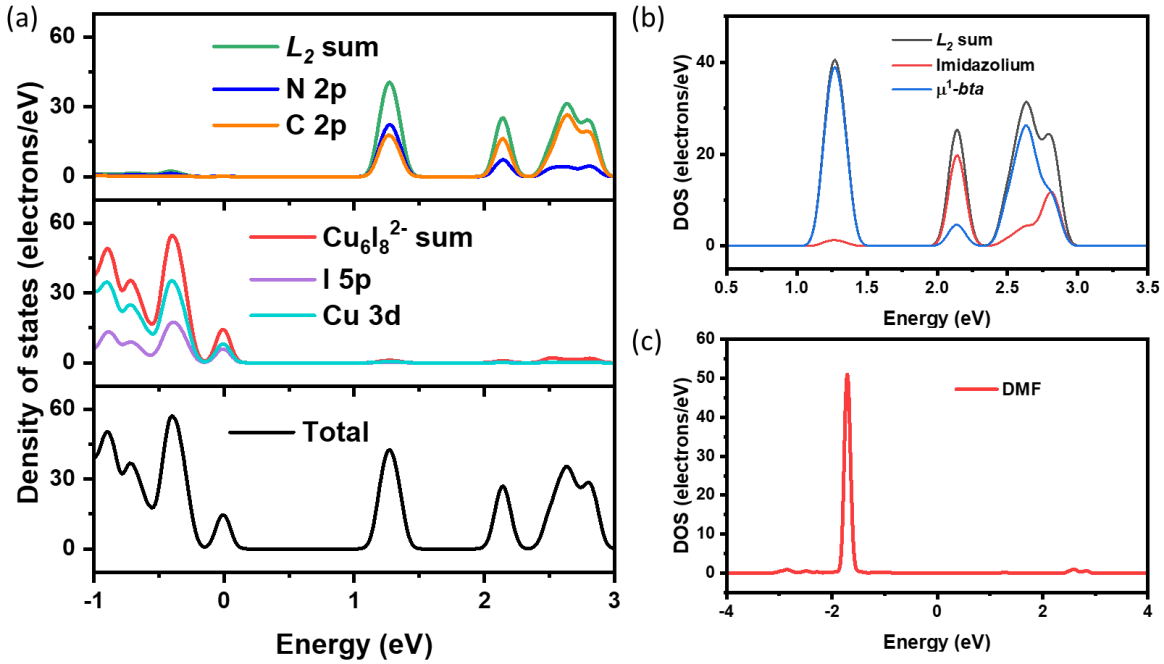


Figure S17. (a) Calculated TDOS and PDOS of compound **3**. (b) Zoom in of the conduction band region of compound **3**. (c) Contributions from solvated DMF molecules.

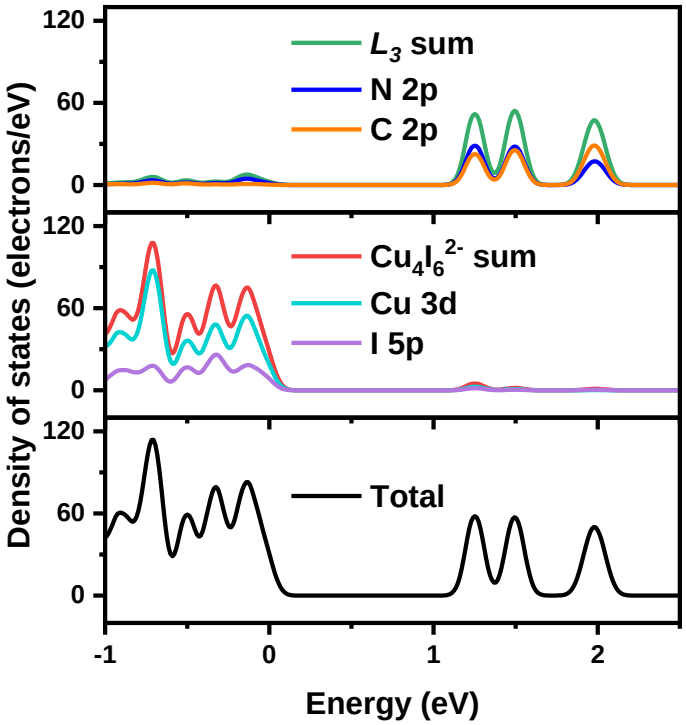


Figure S18. (a) Calculated TDOS and PDOS of compound **4**.

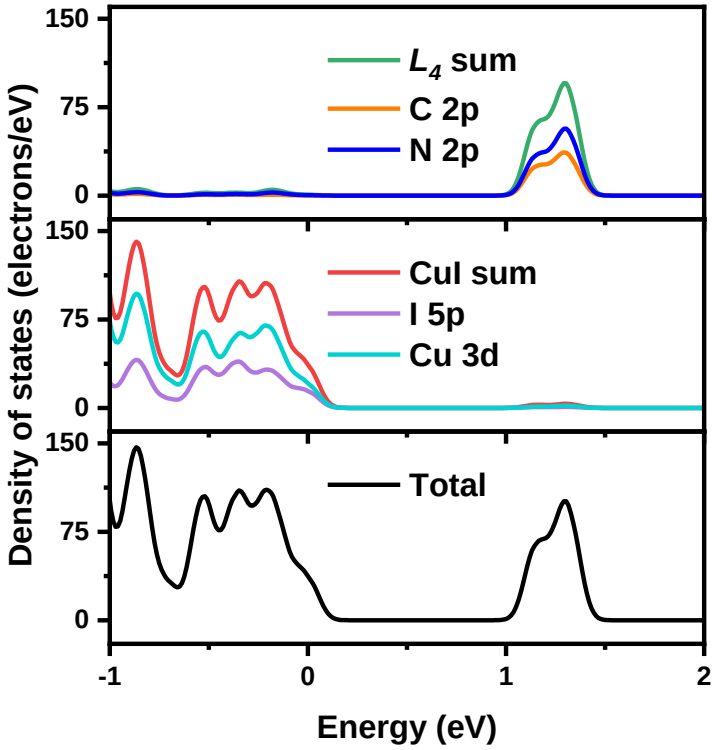


Figure S19. (a) Calculated TDOS and PDOS of compound **5**.